

Synthesis and structure of a stuffed derivative of α -quartz, $\text{Mg}_{0.5}\text{AlSiO}_4$

HONGWU XU,^{1,*} PETER J. HEANEY,² PING YU³ AND HUIFANG XU⁴

¹Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, U.S.A.

²Department of Geosciences, Pennsylvania State University, University Park, Pennsylvania 16802, U.S.A.

³Nuclear Magnetic Resonance Facility, University of California at Davis, Davis, California 95616, U.S.A.

⁴Department of Geoscience, University of Wisconsin, Madison, Wisconsin 53706, U.S.A.

ABSTRACT

A structural derivative of quartz with the composition $\text{Mg}_{0.5}\text{AlSiO}_4$ has been grown from glass and characterized using synchrotron X-ray diffraction (XRD), transmission electron microscopy (TEM), and ^{29}Si nuclear magnetic resonance (NMR) spectroscopy. Rietveld analysis of the XRD data indicates that the framework of $\text{Mg}_{0.5}\text{AlSiO}_4$ is isostructural with α -quartz, rather than β -quartz, as is consistent with previous theoretical modeling (Sternitzke and Müller 1991). Al and Si exhibit long-range disorder over the framework tetrahedral sites, indicated by the absence of the superlattice reflections corresponding to the doubling of c relative to that of quartz. Nevertheless, ^{29}Si NMR measurements show that Al and Si exhibit partial short-range order with an ordering degree of 56%. Electron diffraction reveals superlattice reflections indicative of doubled periodicities along the **a**-axes. Fourier electron density maps show that Mg occupies channel sites that each are bonded to six O atoms, in contrast to the tetrahedral coordination of Li in the β -quartz-type framework for β -eucryptite, LiAlSiO_4 . Furthermore, the concentrations of Mg in adjacent channels are different, resulting in framework distortions that generate the superstructures along **a**.

Keywords: Quartz, eucryptite, stuffed derivative, synthesis, crystal structure, synchrotron X-ray diffraction, transmission electron microscopy, nuclear magnetic resonance spectroscopy